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Addition/Correction

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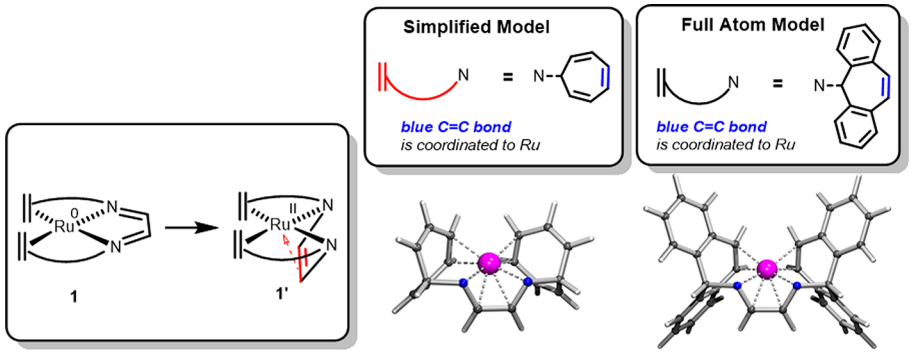
Correction to "DFT Provides Insight into the Additive-Free Conversion of Aqueous Methanol to Dihydrogen Catalyzed by [Ru(trop$_2$dad)]: Importance of the (Electronic) Flexibility of the Diazadiene Moiety"

Vivek Sinha, Monica Trincado, Hansjörg Grützmacher,* and Bas de Bruin*

J. Am. Chem. Soc. **2018**, *140*, 13103−13114. DOI: 10.1021/jacs.8b09011

Pages 13107 and 13110. During the proof correction process, the Figure 3 graphic was incorrectly replaced with a higher-resolution image that was intended to replace the Figure 6 graphic. The correct figures are shown here.



Method	Relative energy of 1′$_{simplified}$ with respect to complex 1$_{simplified}$ (*kcal mol^{-1}*)	Relative energy of 1′ with respect to complex 1 (full-atom model) (*kcal mol^{-1}*)
BP86//B3LYP (gas phase)	**+8.1**	**+3.9**
BP86//B3LYP (Water)	**+7.2**	**+3.4**
BP86//B3LYP (THF)	**+7.5**	**+3.5**
BP86//M06 (gas phase)	**+6.2**	**+1.6**
BP86//M06 (Water)	**+5.1**	**+1.0**
BP86//M06 (THF)	**+5.4**	**+1.2**
BP86 (gas phase)	**+10.2**	**+5.9**

Figure 3. Comparison of relative stabilities (computed Gibbs free energy at 298 K) of complexes **1′** and **1** with full-atom and simplified models.

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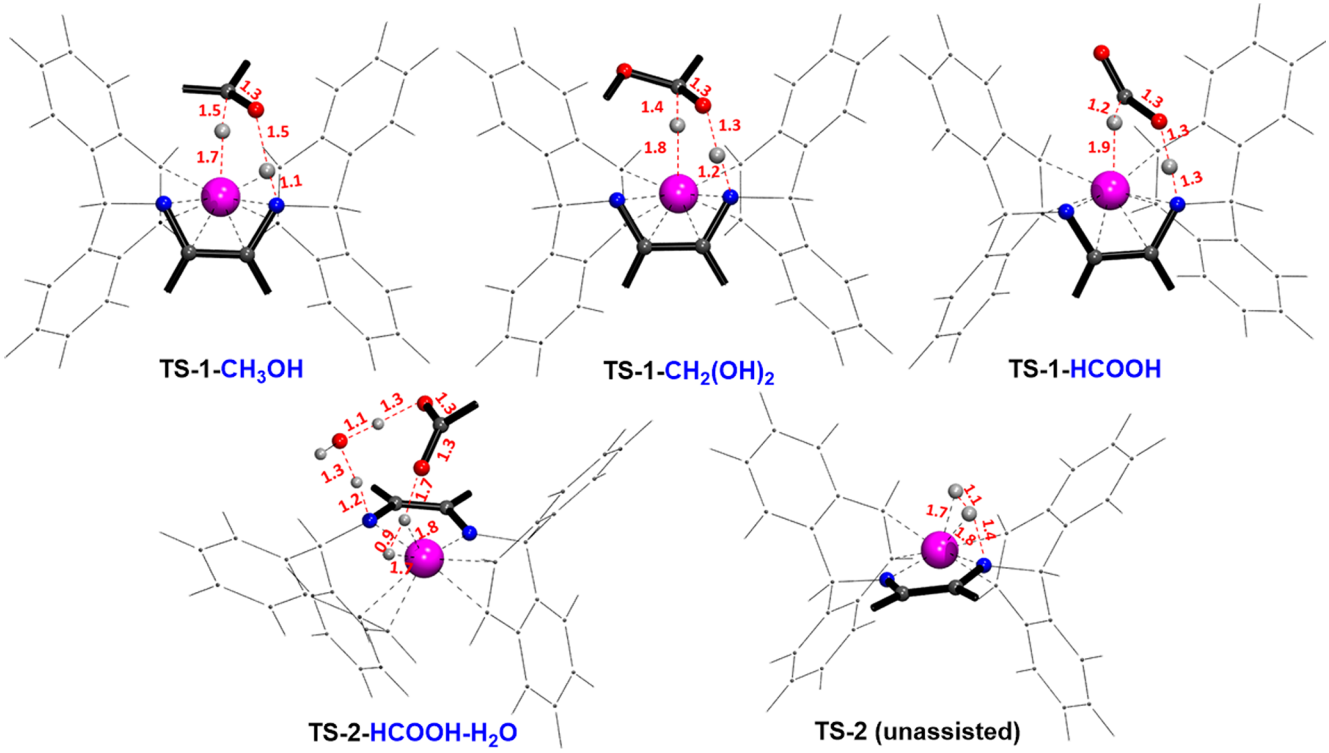

Figure 6. Snapshots of optimized geometries of the transition states reported in the main text along with relevant bond lengths (in Å).

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